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## COMPLETED PROJECT SUMMARY

1. **TITLE:** Resonant Charge Exchange Studies with Hyperthermal Energy Ion Beams:  
Development of multi-detection capabilities and a data acquisition system.
2. **PRINCIPAL INVESTIGATOR:** Dr. Barbara H. Cooper  
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David M. Goodstein  
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  1. "An Efficient Algorithm for the Simulation of Hyperthermal Energy Ion Scattering", D.M. Goodstein, S.A. Langer, and B.H. Cooper, J. Vac. Sci. Tech., A 6(3), 703 (1988).
  2. "The Design and Performance of a UHV Beamline to Produce Low and Hyperthermal Energy Ion Beams", D.L. Adler and B.H. Cooper, Rev. Sci. Instrum., 59, 137 (1988).
  3. "Design and Performance of Ion Optics for Hyperthermal (10-100 eV) and keV Ion Scattering", D.L. Adler, B.H. Cooper, and D.R. Peale, J. Vac. Sci. Tech., A 6(3), 804 (1988).
  4. "A Versatile Apparatus for Low Energy and Hyperthermal Energy Ion Scattering Spectroscopy", R.L. McEachern, D.L. Adler, D.M. Goodstein, G.A. Kimmel, B.R. Litt, D.R. Peale, and B.H. Cooper, Rev. Sci. Instrum., in press.
  5. "A Source for Producing Alkali Ion Beams for Low Energy Surface Scattering Spectroscopies", D.R. Peale, D.L. Adler, B.R. Litt, and B.H. Cooper, submitted to Rev. Sci. Instrum. (1988).
  6. "Trajectory Analysis of Low Energy and Hyperthermal Ions Scattered from Cu(110)", R.L. McEachern, D.M. Goodstein, and B.H. Cooper, submitted to Phys. Rev. B (1988).

7. "Low Energy Alkali Ion Scattering as a Probe of Resonant Charge Exchange on Cesium Cu(110)", G.A. Kimmel, D.M. Goodstein, and B.H. Cooper, submitted to J. Vac. Sci. Tech., AVS conference proceedings (1988).
8. "Hartree-Fock Potentials for Alkali Ion-Metal Scattering Below 500 eV", D.M. Goodstein, R.L. McEachern, and B.H. Cooper, in preparation (1988).
9. "Rainbow Scattering for 100 to 400 eV Na<sup>+</sup> from Cu(110)", D.L. Adler, R.L. McEachern, D.M. Goodstein, and B.H. Cooper, in preparation (1988).
10. "Resonant Charge Exchange Studies with Hyperthermal Energy Ion Beams: Development of multi-detection capabilities and a data acquisition system", B.H. Cooper, Final Technical Report to AFOSR (1988).

## 9. ABSTRACT OF OBJECTIVES AND ACCOMPLISHMENTS:

The present grant (AFOSR-87-0048) is for design and construction of instrumentation to be used for research supported by the Air Force (presently funded under grant AFOSR-88-0069).

The objectives of the instrumentation development were to complete the overall apparatus, to design and construct multi-detectors for the scattered ions, and to configure a computer system that could handle real-time data acquisition from the multi-detectors.

Progress in instrumentation includes: the successful production of low phase-space alkali and noble gas beams ranging in energy from  $\approx 10$  eV to several keV, completion of two hemispherical analyzers for detecting scattered ions (one with high-resolution capabilities, the other for large angle scattering studies), position-sensitive pulse-counting detectors for multi-energy detection, and a Macintosh II-based data acquisition system which receives and stores data from the storage buffers of the multi-detectors.

The scientific objectives are to investigate the interactions of hyperthermal (10-100 eV) and keV ions with metal surfaces. Particular emphasis is placed on the study of ion-surface charge transfer processes.

Scientific progress includes: measurements of 50 eV to 4 keV alkali scattering from clean and cesiated-Cu(110), simulations using Hartree-Fock pair potentials that give good agreement with the 100 to 400 eV Na<sup>+</sup> scattering from Cu(110), trajectory analysis to identify peaks in the Na<sup>+</sup> energy spectra, measurements of charge transfer probabilities for alkalis scattered from Cu(110) with low coverages ( $< 1/10$  monolayer) of Cs adsorbates, and ongoing development of a model that includes both local and collective effects of the Cs adsorbates in determining charge transfer probabilities.

AFOSR Program Manager:  
Larry W. Burggraf, Lt Col, USAF

Report: Grant no. AFOSR-87-0048

# RESONANT CHARGE EXCHANGE STUDIES WITH HYPERTHERMAL ENERGY ION BEAMS

Development of Multi-Detection Capabilities and a Data Acquisition System

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## INTRODUCTION

Grant no. AFOSR-87-0048 was solely for instrumentation development and construction. Personnel, operating costs, and further hardware for this research program have been funded by AFOSR-86-0086 (1 April 1986 to 15 November 1987) and are currently funded under AFOSR-88-0069 (starting data 15 November 1987). Progress on instrumentation development and construction is given in this report. Scientific progress for the whole research program will be briefly summarized; more information was given in the final technical report for AFOSR-86-0086.

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## I. SUMMARY

The overall research program described in this report is to investigate the interactions of hyperthermal energy (10-100eV) and low energy (keV) ions with clean and adsorbate-covered metal surfaces. A particular emphasis is placed on the study of ion-surface charge exchange processes.

The following results are reported:

- 1) Completion and performance of the apparatus for low and hyperthermal energy ion scattering.
  - a) General completion of the apparatus.
  - b) Completion of the construction of two hemispherical electrostatic analyzers, and associated position-sensitive sensors and pulse-counting electronics for detecting scattered ions in the multi-energy-channel mode.
  - c) Configuration of a Macintosh II-based data acquisition system which will receive and store data from the storage buffers of the multi-detectors.
- 2) Status report of the scientific progress for research funded by the AFOSR.

Included is a brief description of alkali ion (lithium, sodium and potassium) scattering measurements from clean and cesiated copper surfaces. Specific results are reported on ion-surface interaction potentials and trajectory analysis for 100 to 400 eV sodium ion scattering from clean Cu(110). Also reported are measurements of resonant charge transfer probabilities for alkalis scattered from Cu(110) surfaces with low coverages ( $<1/10$  of a monolayer) of cesium adsorbates.

## II. RESEARCH OBJECTIVES

The present grant (AFOSR-87-0048) is for design and construction of instrumentation to be used for research supported by the Air Force (presently funded under grant AFOSR-88-0069).

The objectives of the instrumentation development were to design and construct multi-detectors for the scattered ions and to configure a computer system that could handle real-time data acquisition from the multi-detectors. We have received all the hardware and electronics covered by AFOSR-87-0048; details of the final configurations are reported below.

Scientific objectives are to investigate the interactions of hyperthermal (10-100 eV) and keV ions with metal surfaces. Specific experimental goals are:

1. To investigate ion-surface interaction potentials that accurately describe scattering at hyperthermal energies.
2. To analyze hyperthermal energy ion-surface scattering trajectories and kinematics.
3. To measure ion-surface charge transfer probabilities in order to probe the mechanisms of resonant single-electron charge transfer.
4. To combine the information in 1,2, and 3 above in order to develop a microscopic picture of resonant charge transfer in low energy and hyperthermal energy ion-surface scattering, and to understand the role of low-coverage adsorbates in determining these charge transfer rates.

Results of these experiments are also given very briefly below.

## III. STATUS OF RESEARCH

### 1) Completion and Performance of Apparatus

#### a) General completion of apparatus

We have recently completed construction of a UHV scattering chamber for ion beam analysis of single crystal surfaces [1]. The beams range in energy from  $\approx 10$  eV to 10 keV. Available beams include alkali ions, noble gases, and other gas atomic and molecular species. Full energy- and angle-resolved spectra of scattered ions are measured using electrostatic analyzers and pulse-counting electronics; these detectors are being upgraded to the multi-channel mode. Additional capabilities include Auger electron spectroscopy, low energy electron diffraction, sputter cleaning and annealing, and hardware for gas and alkali atom deposition. We have added to the chamber a Kelvin probe for making work function measurements and hardware for thermal desorption spectroscopy. We have also installed a new sample manipulator with heating and cooling capabilities and a vacuum sample transfer system. More detail on the ion scattering hardware, in particular the multi-detectors and the data acquisition system, are given below.

#### b) Beamline and source

Making use of two different ion optics and transport programs, we have designed a differentially-pumped UHV system to produce well-characterized singly-ionized beams of

alkali and noble gas ions in the energy range from  $\sim 10$  eV to 10 keV [2]. Beam transport was designed to minimize the effects of space charge spreading for the hyperthermal energy beams. For producing the alkali ion beams, we have recently completed construction of a source with high extraction efficiency [3]. The extraction electrodes are based on a modified Pierce geometry. The source uses a solid state alkali ion emitter (made by Spectra Mat, Inc.) and two stages of extraction. A wire mesh in the first stage produces a uniform current density across the beam profile. Using this source we can produce beams of Li, Na, K, Rb, and Cs ions.

We can now routinely produce low phase space alkali and noble gas beams. Above a few hundred eV the beam diameter at the sample position is on the order of 1 mm and the angular divergence of the beam is  $< 1^\circ$ . A typical 100 eV beam has a diameter of  $\approx 3$  mm, an angular divergence of  $\pm 1 - 2^\circ$ , and a current of several nanoamps. Beams of 50 eV and lower have slightly larger diameters and angular divergences, but have similar currents of several nanoamps. More details of the beam profiles are given in ref 2.

### c) Multi-channel electrostatic analyzers and electronics

The detector for the scattered ions is a hemispherical electrostatic analyzer with a 50 mm mean radius. The gap is 35% of the mean radius. One mm input and output apertures define the energy resolution to be 1% of the pass energy.

Two sets of electronics are used with this analyzer. The first is a set of low voltage electronics which is used for the hyperthermal energy beams (for pass energies of 0-170 eV). The other is a set of high voltage electronics used for pass energies of  $\sim 100$  eV to 10 keV. The analyzer is designed so that the desired pass energy is chosen by putting equal and opposite voltages on the two hemispheres. An energy scan is taken by sweeping the potential on the hemispheres under computer control with programmable dwell time and a programmable number of repetitive sweeps.

Currently the analyzer is equipped with a Channeltron electron multiplier for counting the energy-analyzed ions. The multiplier can be used in either the pulse-counting or analog mode. Counts are accepted from the electron multiplier using a computer-interfaced scaler with programmable dwell times.

Ions with a substantial range of energies are dispersed across the gap between the hemispheres of the detector. To minimize the collection time and total beam dose required to measure a given energy spectrum, the aperture and Channeltron at the exit of the 50 mm analyzer will be replaced with a position-sensitive detector (Surface Science Laboratories Model 3390A). This consists of two microchannel plate electron multipliers mounted in front of a resistive anode encoder. The sensor has a 25-mm-diameter circular active area, spatial resolution of 100 line pairs, and is fully UHV compatible. The position computing electronics (Surface Science Laboratories Model 2401A) can calculate the position of a pulse in 3  $\mu$ s, providing the information as an 8-bit word for each dimension. An internal buffer stores 12 bits of information for each pulse (e.g. 8 bits of one dimension, 4 of the other). The stored data can be sent to the computer via a parallel interface while new data are being accumulated. Count rates in excess of 100 kHz are possible with negligible pile-up error; however, considering the angular resolution of the detector and our typical beam currents, we will not exceed a few tens of kHz. Based on the geometry of our analyzer,

we expect to achieve approximately an order of magnitude reduction in data collection time. We have received delivery on the hardware and electronics for the multi-detection upgrade.

We have also considered the use of a toroidal geometry analyzer as a multi-channel detector. The toroidal analyzer can be used to disperse ions with different energies and angles in a two-dimensional array at the output plane. The toroidal analyzers currently in use in other laboratories use relatively small gaps between the sectors, resulting in detection of scattered ions over a broad angular range, but restricted to a relatively small range of energies. At the present time, most of our research requires scanning broad ranges of scattered energies; the spectral features generally do not vary rapidly with angle. For that reason we are using the 50 mm spherical analyzer in the multi-detection mode, and are investigating the use of a large-gap toroidal analyzer for future use.

Due to the relatively large size of our present 50 mm analyzer and due to space constraints inside the scattering chamber, the largest scattering angle accessible with the present arrangement is  $128^\circ$ . In order to detect scattered ions at angles near  $180^\circ$ , we have built a spherical analyzer which is a half-size version of the 50 mm analyzer. Grooves cut into the spherical surfaces help to keep particles which scatter off the inner surfaces of the analyzer from being counted in the electron multiplier. The new 25 mm analyzer is also equipped with a resistive anode for multi-energy detection.

Under grant AFOSR-88-0069 we are constructing a new chamber for sample preparation and analysis. The new chamber will house a scanning tunneling microscope (STM) and provisions for ion scattering. Since only one ion detector is needed at a given time per chamber, eventually each of the chambers (the existing one and the one under construction) will be equipped with one of the multi-detectors described above. One of these systems will be better suited for high-resolution energy scans (50 mm analyzer) and the other for large-angle backscattering studies (25 mm analyzer), which are particularly useful for determining local structures at surfaces.

### c) Data acquisition system

Using funds from this grant we have purchased a Macintosh II computer with a 19" color graphics monitor. Via parallel interfaces, the computer will be used to receive and store data from the storage buffers of the multi-detectors. The Macintosh II will also serve as the data acquisition and display system for the STM.

## 2) Status of Scientific Results

Measurements of 50 eV to 4 keV alkali ( $K^+$ ,  $Na^+$ , and  $Li^+$ ) scattering from Cu(110) have been completed. Using our computer code SAFARI [4], we have made significant progress toward successful simulation of hyperthermal energy alkali ion scattering. We have analyzed the energy spectra from the Cu(110) surface along both the  $\langle 001 \rangle$  and  $\langle 1\bar{1}0 \rangle$  azimuths with beams of 4 keV, 1 keV, 400 eV, 200 eV, 100 eV, and 50 eV incident energies. Using the simulation we get very good agreement with our measured energy spectra for the 100, 200, and 400 eV  $Na^+$  beams. The potential used in these simulations is a sum of  $Na^+/Cu$  pair potentials, with an added image potential which depends only



on distance from the surface. The pair potential is a sum of two exponential terms (with four parameters). The four parameters were chosen to fit a  $\text{Na}^+/\text{Cu}$  dimer calculation within the Hartree-Fock approximation. We are extending this work now to the  $\text{K}^+$  and  $\text{Li}^+$  spectra [5].

Some very interesting energy-dependent trends in peak positions and intensities have appeared when we compare the  $\text{Na}^+$  scattering in the two azimuths as the beam energy is varied from 50 eV to 4 keV. Using trajectory analysis from the SAFARI simulations, we have been able to correlate these trends with particular types of trajectories whose positions in the spectra vary with the incident beam energy [6]. We are also analyzing the angular features of the scattering, in particular the positions of the rainbow angles, which are very sensitive to details of the potential [7].

Charge transfer probabilities have been measured for alkali scattering from  $\text{Cu}(110)$  with low coverages ( $<1/10$  monolayer) of Cs adsorbates. The functional form of the measured scattered-ion intensity decrease with decreasing work function (increasing Cs coverage) indicates that the effect of the Cs adsorbates cannot be described as a uniform shift in the surface work function [8]. We are working on a model that includes both local and collective effects of the adsorbates on the charge transfer process. Results from the studies of the interaction potentials and the scattered ion trajectory analyses will enable us to examine the charge transfer as a function of individual types of trajectories at the surface.

#### IV. REFERENCES

- [1] R.L. McEachern, D.L. Adler, D.M. Goodstein, G.A. Kimmel, B.R. Litt, D.R. Peale, and B.H. Cooper, *Rev. Sci. Instrum.*, in press.
- [2] D.L. Adler and B.H. Cooper, *Rev. Sci. Instrum.*, **59**, 137 (1988).
- [3] D.R. Peale, D.L. Adler, B.R. Litt, and B.H. Cooper, submitted for publication (1988).
- [4] D.M. Goodstein, S.A. Langer, and B.H. Cooper, *J. Vac. Sci. Tech., A* **6**(3), 703 (1988).
- [5] D.M. Goodstein, R.L. McEachern, and B.H. Cooper, in preparation (1988).
- [6] R.L. McEachern, D.M. Goodstein, and B.H. Cooper, submitted for publication (1988).
- [7] D.L. Adler, R.L. McEachern, D.M. Goodstein, and B.H. Cooper, in preparation (1988).
- [8] G.A. Kimmel, D.M. Goodstein, and B.H. Cooper, submitted for publication (1988).

#### V. RESEARCH PARTICIPANTS

Participating in the charge exchange research program are myself (partial summer salary from AFOSR-88-0069) and graduate students D.M. Goodstein and D.R. Peale (both supported by AFOSR-88-0069). Other students working on the apparatus and involved in related research programs are G.A. Kimmel (also working on charge transfer experiments), R.L. McEachern, and E. Behringer (supported by PYI/NSF-DMR-8451979), D.L. Adler (supported by MSC/NSF-DMR-8516616), and C. DiRubio.

## VI. PUBLICATIONS

- 1) An Efficient Algorithm for the Simulation of Hyperthermal Energy Ion Scattering,  
David M. Goodstein, Stephen A. Langer, and B.H. Cooper, J. Vac. Sci. Tech.,  
A 6(3), 703 (1988).
- 2) The Design and Performance of a UHV Beamline to Produce Low and Hyperthermal  
Energy Ion Beams,  
D.L. Adler and B.H. Cooper, Rev. Sci. Instrum., 59, 137 (1988).
- 3) Design and Performance of Ion Optics for Hyperthermal (10-100 eV) and keV Ion  
Scattering,  
D.L. Adler, B.H. Cooper, and D.R. Peale, J. Vac. Sci. Tech., A 6(3), 804 (1988).

The following papers have been accepted for publication:

- 4) A Versatile Apparatus for Low Energy and Hyperthermal Energy Ion Scattering Spec-  
troscopy,  
R.L. McEachern, D.L. Adler, D.M. Goodstein, G.A. Kimmel, B.R. Litt, D.R.  
Peale, and B.H. Cooper, Rev. Sci. Instrum., in press.

The following papers are submitted for publication:

- 5) A Source for Producing Alkali Ion Beams for Low Energy Surface Scattering Spectro-  
scopies,  
D.R. Peale, D.L. Adler, B.R. Litt, and B.H. Cooper, submitted to Rev. Sci.  
Instrum. (1988).
- 6) Trajectory Analysis of Low Energy and Hyperthermal Ions Scattered from Cu(110),  
R.L. McEachern, D.M. Goodstein, and B.H. Cooper, submitted to Phys. Rev. B  
(1988).
- 7) Low Energy Alkali Ion Scattering as a Probe of Resonant Charge Exchange on Cesi-  
ated Cu(110),  
G.A. Kimmel, D.M. Goodstein, and B.H. Cooper, submitted to J. Vac. Sci. Tech.  
(1988), AVS 1988 conference proceedings.

The following papers are in preparation:

- 8) Hartree-Fock Potentials for Alkali Ion-Metal Scattering Below 500 eV,  
D.M. Goodstein, R.L. McEachern, and B.H. Cooper, in preparation (1988).
- 9) Rainbow Scattering for 100 to 400 eV Na<sup>+</sup> from Cu(110),  
D.L. Adler, R.L. McEachern, D.M. Goodstein, and B.H. Cooper, in preparation  
(1988).

## VII. PRESENTATIONS

- 1) Computer Simulations of Hyperthermal Ion Scattering: Measuring Short-Range Surface Order in Crystals,  
B .H. Cooper and D.M. Goodstein, presented at the Sixth International Workshop on Inelastic Ion Surface Collisions, Argonne National Laboratory, August 1986.
- 2) Hyperthermal Ion-Surface Scattering Simulation: Alternatives to Monte Carlo,  
D.M. Goodstein, S.A. Langer, and B.H. Cooper, presented at the New York Meeting of the American Physical Society, March 1987.
- 3) A Versatile Apparatus for Low Energy and Hyperthermal Ion Scattering,  
R.L. McEachern and B.H. Cooper, presented at the New York meeting of the American Physical Society, March 1987.
- 4) An Ion Scattering System for the Energy Range 10eV to 10keV,  
D.L. Adler and B.H. Cooper, presented at the New York meeting of the American Physical Society, March 1987.
- 5) Ion-Surface Scattering at Low and Hyperthermal Energies: Scattering Dynamics and Charge Exchange in Relation to Surface Chemistry,  
B.H. Cooper, invited talk at the American Chemical Society Meeting, New Orleans, September 1987.
- 6) Ion Surface Scattering at Hyperthermal Energies: Scattering Dynamics and Charge Exchange,  
B.H. Cooper, talk at the AFOSR Surface Chemistry Contractor's Conference, Colorado Springs, September 1987.
- 7) Interactions of Hyperthermal Ion Beams with Metal Surfaces,  
D.M. Goodstein, R.L. McEachern, and B.H. Cooper, presented at the 34<sup>th</sup> National Symposium of the American Vacuum Society, Anaheim, California, November 1987.
- 8) Design and Performance of Ion Optics for Hyperthermal (10-100 eV) and keV Ion Scattering,  
D.L. Adler, B.H. Cooper, and D.R. Peale, presented at the 34<sup>th</sup> National Symposium of the American Vacuum Society, Anaheim, California, November 1987.
- 9) Scattering Dynamics of Low Energy Alkali and Noble Gas Ions Incident on Cu(110),  
R.L. McEachern, D.L. Adler, D.M. Goodstein, G.A. Kimmel, and B.H. Cooper, presented at the New Orleans meeting of the American Physical Society, March 1988.
- 10) Low Energy Ion Scattering Studies of Surfaces Disordered by Ion Bombardment,  
G.A. Kimmel, D.L. Adler, D.M. Goodstein, R.L. McEachern, and B.H. Cooper, presented at the New Orleans meeting of the American Physical Society, March 1988.

- 11) Structural Study of the O/Cu(110) System Using Hyperthermal and Low Energy Noble Gas and Alkali Ion Scattering,  
D.L. Adler, R.L. McEachern, D.M. Goodstein, G.A. Kimmel, and B.H. Cooper, presented at the New Orleans meeting of the American Physical Society, March 1988.
- 12) Hyperthermal Alkali Ion Scattering from Cu(110),  
D.M. Goodstein, D.L. Adler, R.L. McEachern, and B.H. Cooper, presented at the New Orleans meeting of the American Physical Society, March 1988.
- 13) Low and Hyperthermal Energy Ion-Surface Scattering: Trajectory Analysis, Multiple Scattering, and Charge Exchange,  
B.H. Cooper, invited talk at Rutgers University, Piscataway, NJ, April 1988.
- 14) Scattering of 50 eV to 4 keV Alkali Ion Beams from Cu(110) Surfaces: Trajectory Analysis and Charge Exchange,  
B.H. Cooper, invited talk at Xerox Corporation, Webster, NY, June 1988.
- 15) Ion-Surface Scattering at Hyperthermal and keV Energies: Interaction Potentials, Trajectory Analysis, and Charge Exchange,  
B.H. Cooper, talk at the 48<sup>th</sup> Annual Conference on Physical Electronics, Brookhaven Labs, June 1988.